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Final Technical Report

Mathematical Prediction of the Physical Properties
of Materials and Media:
Grant #F49620-96-1-0008

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OBJECTIVES

- * Application of the method of boundary variations to the calculation of electromagnetic scattering by three-dimensional bounded obstacles
- * Development of fast high-order integral methods for solution of problems of electromagnetic scattering involving surface and volume integrals
- * Description, based on homogenization and nonlinear elasticity theory, of conservative and dissipative mechanisms associated to the shape memory effect and hysteresis in Shape Memory Alloys.

BOUNDARY VARIATIONS

A fully three-dimensional boundary-variations code for the Helmholtz equation was developed and tested (in collaboration with F. Reitich); numerical results show excellent accuracy's for large departures from spherical shapes, in line with those obtained for diffraction gratings. Numerical results of this code were described in the article "Boundary-variation solutions for bounded-obstacle scattering problems in three dimensions".

As an additional application of the method of variation of boundaries we introduced (in collaboration with A. Sei and M. Caponi) a theory on the occurrence of sea-spikes in electromagnetic scattering from the ocean, based on certain strong anomalies we encountered which we called Non-Rayleigh Anomalies. The resulting paper has now been accepted for publication in the journal Radio Science. We believe this work clears a controversy which has stood for a period of some 50 years. This work was motivated through our recent collaboration with a team of TRW scientists whose expertise lies on experiment and theory on scattering from the ocean. Over the summer M. Caponi, A. Sei and I have been collaborating with a

Caltech undergraduate student, Peter Stobbe (under support of TRW). Peter has been running a variety of statistical tests on our Boundary Variations code, to insure that the anomalies we have discovered continue to occur in a random setting. He has confirmed that they do, according to our expectations.

Over the last few months, again motivated by interests of TRW as well as the Air Force (as expressed in a Hanscomb meeting on rough surfaces) Alain Sei and I have been developing a numerical method for the solution of EM scattering problems involving multiple-scale scatterers. Our overall approach is, again, based on boundary variation methods. At this time we are focusing on finding solutions required by our boundary variations approach, namely, to obtain a high-frequency expansion of the scattering solutions.

In a final effort on Boundary Variation methods we are pursuing, in collaboration with F. Reitich, an extension of our approach for the solution of eigenvalue-type problems. We currently have running a test code which solves eigenvalue problems in perturbed geometries. The actual problem of interest, the whispering gallery modes, is a closely related transmission eigenvalue-like problem which will be treated in the near future. One of the main difficulties in developing our eigenvalue code was to derive a recursive relation for the successive terms in the perturbation series. This difficulty arose as a result of the possible existence of multiple eigenvalues for the unperturbed configuration which continue analytically as separated, distinct eigenvalues. Our focus in the near term will be to complete our theory, complete numerical experiments on our code (which is already running and producing correct results), and to extend this eigenvalue solver to the configurations usually considered in optics: transmission eigenvalue-problems.

FAST INTEGRAL EQUATION SOLVERS

In collaboration with A. Sei, we have developed a new numerical method for solution of problems of scattering by general heterogeneous bodies as presented in "A fast high-order solver for problems of scattering by heterogeneous bodies"; this article has been submitted for publication in IEEE antenn. propag. A student in our department, McKay Hyde (under support of an AASERT AFOSR grant), has taken up this effort. Together with him and with an undergraduate student I hired over the summer, Mike Fisher, we have already introduced substantial improvements to that method, leading to important improvements in the running times. These improvements relate to the method of radial integration we use. In the previous work with Sei the radial integrations were performed by means of suitable interpolations by polynomials; we have now realized that a much better approach can be based on Fourier approximations and the FFT; an idea which resulted from an attempt to obtain very high order integration rules through use of the trapezoidal rule. The trapezoidal rule is exponentially convergent for periodic

analytic functions, but it exhibits very low order convergence for non-periodic functions. What we have accomplished is to provide a "high order trapezoidal rule for non-periodic functions", which works through consideration of FFT's. (Recall that consideration of Fourier series lies at the basis of the exponential convergence of the trapezoidal rule for periodic functions). We consider this an important breakthrough, and we are looking forward to many applications of this method.

In a related effort I am conducting weekly meetings with Chuck Molloy (from Lockheed Martin Skunk Works, Palmdale) and investigating matters relevant to Lockheed's interests (under a consulting agreement between my new company, MathSys, and Lockheed) on extending our fast methods as described above to problems of scattering by surfaces in three dimensional space. I expect my forthcoming postdoctoral associate Leonid Kunyansky, under support of AFOSR, will join me in my efforts to extend our fast methods to this case.

MICROSTRUCTURES, PHASE TRANSITIONS IN SOLIDS, MAGNETIC MATERIALS

In the area of solid-to-solid phase transitions I have studied, in collaboration with Guillermo Goldsztein (under support of NSF) the problem of elasticity in polycrystals that arises as shape deforming phase transitions give rise to misfits in polycrystalline solids. Our results provide a fast method (of order $O(N)$ where N is the number of grains) for the computation of the overall elastic energy in two- and three-dimensional polycrystals (!). In a related effort, in collaboration with Liliana Borcea (our former postdoc, former student of G. Papanicolaou, now assistant professor at the department of applied math at Rice) we are developing methods for the solution of problems of magnetoelasticity. This effort is reaching maturity at this point, with a fully developed theory on elastomers, and a code to predict the overall properties of magneto-elastomers and magneto-rheological fluids will be in place soon.

A related but different effort will be initiated (under support of DOE-ASCI) in collaboration with my forthcoming postdoctoral associate Dimitri Vaynblat, a recent graduate from MIT math. Our focus will be on phase transition in solids under shock conditions. This is the kind of situation which gives rise to phase transitions such as graphite-to-diamond or between various phases of iron. Our effort will draw from recent work of ours on dynamic phase transitions (with Leo and Shield, with Leo and Reitich, as well as work of my own), and it will incorporate new aspects relating to the high-pressure aspects of this present problem.

PUBLICATIONS RESULTING FROM THIS AWARD

- [1] Calculation of electromagnetic scattering via boundary variations and analytic continuation, O. P. Bruno and F. Reitich, *ACES Jour.* 11 (1996), 17--31
- [2] On the MHD equations in a three dimensional toroidal geometry, O. Bruno and P. Laurence, *Comm. Pure Appl. Math.* 49(1996), 717--764
- [3] The overall elastic energy of polycrystalline martensitic solids, O. Bruno, F. Reitich and P. H. Leo, *J. Mech. Phys. Solids* 44(1996), 1051--1101
- [4] Energetics in martensites, O. Bruno, *Solid Mechanics and its Applications* 60, pp. 91-108, 1998.
- [5] Shape deforming phase transitions in solids: energetics and pseudoelasticity, O. Bruno, *Solid Mechanics and its Applications* 62, pp. 319-324, 1998.
- [6] Boundary-variation solutions in problems of scattering by three dimensional bounded obstacles, O. P. Bruno and F. Reitich, *J. Acous. Soc. Amer.* 104, pp 2579-2583, 1998
- [7] Bounds on the effective elastic properties of martensitic polycrystals, O. P. Bruno and F. Reitich, in "Mathematics of Multiscale Materials", Golden, Grimmer, James, Milton, Sen, Eds. (1998) pp. 51-62.
- [8] Study of polarization dependent scattering anomalies with applications to oceanic scattering, A. Sei, O. Bruno and M. Caponi, to appear in *Radio Science*
- [9] A fast high-order solver for problems of scattering by heterogeneous bodies, O. Bruno and A. Sei, Submitted to *IEEE Antenn. Propag.*
- [10] Two-wave structures in shock-induced martensitic phase transitions, O. Bruno and D. Vaynblat, Submitted to *Phys. Rev. Lett.*
- [11] A fast algorithm for the simulation of polycrystalline misfits: martensitic transformations in two space dimensions, O. Bruno and G. Goldsztein, Submitted to *J. Mech. Phys. Solids*
- [12] Numerical simulation of martensitic transformations in two- and three-dimensional polycrystals, O. Bruno and G. Goldsztein, Submitted to *J. Mech. Phys. Solids*

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